How to prepare quantum states that follow classical paths

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Abstract

We present an alternative quantization procedure for the one-dimensional non-relativistic quantum mechanics. We show that, for the case of a free particle and a particle in a box, the complete classical and quantum correspondence can be obtained using this formulation. The resulting wave packets do not disperse and strongly peak on the classical paths. Moreover, for the case of the free particle, they satisfy minimum uncertainty relation.

Keywords: Quantum mechanics; Classical-quantum correspondence; Wave packets.

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1 Introduction

Schrödinger equation $H\psi = i\hbar\dot{\psi}$ is the main equation of non-relativistic quantum physics which can be obtained upon the quantization procedure $\vec{p} \rightarrow -i\hbar\vec{\nabla}$ and $H \rightarrow i\hbar\partial_t$ in the Hamiltonian formulation of quantum mechanics [1, 2]. In fact, this equation determines the time evolution of the particle's wave function. Often, we are interested to find solutions in such a way that they follow the classical trajectories without dispersion and peak on them. But, the construction of such kind of wave packets, except for the case of the simple harmonic oscillator, is not an easy task. For instance, for the case of a free particle, the initial wave function disperses quickly as the particle moves.

The problem of classical and quantum correspondence has attracted much attention in the literature [3]. These efforts have begun by Schrödinger [4] and followed by others in the context of the coherent states. These wave packets are specific kind of quantum states that describe a maximal kind of coherence

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and a classical kind of behavior [5]. In quantum physics, we can construct such kind of quantum states by the superposition of the energy eigenstates which would peak around the classical trajectories. But, in most cases, the wave packets do not maintain their shape and eventually disperse.

One possible way to solve this problem is using an alternative quantization method. In fact, we need to change the differential structure of the Schrödinger equation which has a parabolic form. It has been shown that in the context of quantum cosmology, the hyperbolic nature of its main equation gives us the possibility of complete classical and quantum correspondence [6, 7]. So, the resulting wave packets strongly peak on the classical trajectories and never disperse.

Here, we first consider a one-dimensional model in the presence of an external general potential. Then, we use an alternative classical picture which, after quantization, results in a hyperbolic differential equation. For the case of a free particle and a particle in a box, we solve this equation and construct wave packets using appropriate initial conditions. We show that these wave packets follow the classical paths and strongly peak on them in the whole configuration space.

2 The model

Let us consider a harmonic oscillator as a simple example. In the classical domain, this model has a well-known solution $u(t) = A\cos(\omega t + \delta_1)$. Note that, time explicitly appears in this solution which parameterize the temporal behavior of u. To eliminate the explicit presence of t, we can use an another general solution with the same total energy but different phase *i.e.* $v(t) = A\cos(\omega t + \delta_2)$. Now, we can write the variable u in terms of v instead of t, namely

$$u = \cos(\Delta)v \pm \sin(\Delta)\sqrt{A^2 - v^2}, \tag{1}$$

where $\Delta = \delta_1 - \delta_2$ and $-A \leq u, v \leq A$. So, in general, the trajectory is an ellipse which for $\Delta = \pi/2$ represents a circle. This example shows that we can always parameterize the solution in terms of another one which has the same energy but with arbitrary phase shift. Moreover, for each model, the trajectories are unique due to the specific form of the potential.

Since the both solutions have a same energy and obey a same equation of motion we have

$$\begin{cases} \dfrac{p_u^2}{2m} + V(u) = E, \\ \\ \dfrac{p_v^2}{2m} + V(v) = E. \end{cases} \tag{2}$$

Since the right hand sides are equal, we obtain

$$\mathcal{F} \equiv \frac{p_u^2}{2m} - \frac{p_v^2}{2m} + V(u) - V(v) = 0. \tag{3}$$

In the quantum mechanical domain, we need to quantize above equation. The operator $\mathcal{F}$ can be obtained upon quantization procedure $p_u \to -i\hbar\dfrac{\partial}{\partial u}$ and $p_v \to -i\hbar\dfrac{\partial}{\partial v}$. So, we demand that $\mathcal{F}$ annihilate the wave function *i.e.*

$$\mathcal{F}\Psi(u, v) = 0, \tag{4}$$

or, equivalently

$$\left\{ -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial u^2} + \frac{\hbar^2}{2m}\frac{\partial^2}{\partial v^2} + V(u) - V(v) \right\} \Psi(u, v) = 0. \tag{5}$$

Therefore, Eq. (5) is an alternative quantum mechanical equation which has a different structure with respect to the Schrödinger equation, but both explain the same physics.

Although there is no intrinsic preference between these two pictures, the later has some additional advantages. This is due to the hyperbolic form of Eq. (5) which gives us freedom for choosing the initial wave function and its initial slope. On the other hand, the solutions of a hyperbolic equation are usually highly oscillatory. Since the oscillation around the classical paths is not acceptable, we need to choose appropriate initial conditions to guarantee the classical–quantum correspondence.

In the next section, to show the method, we consider the case of a free particle. For this case, the trajectories in both $u - t$ and $u - v$ planes are straight lines. Since Eq. (5) admits solutions which never disperse and strongly peak on the classical paths, we show that the classical and quantum correspondence arises naturally from this formulation.

3 Free particle

For the case of the free particle ($V = 0$), we have

$$\begin{cases} u(t) = \beta_u t + u_0, \\ \\ v(t) = \beta_v t + v_0, \end{cases} \tag{6}$$

where β is the particle's velocity. Since both solutions have a same total energy, we also have $|\beta_u| = |\beta_v|$ which results in $u = \pm v + u_0 \mp v_0$. So, the trajectories are straight lines with unit absolute slope.

It is straightforward to check that, for $V = 0$, $\cos(ku)\cos(kv)$ and $\sin(ku)\sin(kv)$ are the eigenfunctions of Eq. (5). Therefore, the general solution is

$$\begin{aligned} \Psi(u,v) &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} [A(k)\cos(ku)\cos(kv) \\ &+ iB(k)\sin(ku)\sin(kv)]\ dk. \end{aligned} \tag{7}$$

To find the complete form of the wave packet, we need to specify the coefficients $A(k)$ and $B(k)$. These coefficients can be determined from the initial form of the wave packet at $v = 0$

$$\Psi(u,0) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} A(k)\cos(ku)\, dk, \tag{8}$$

$$\left.\frac{\partial \Psi(u,v)}{\partial v}\right|_{v=0} = \frac{i}{\sqrt{2\pi}} \int_{-\infty}^{\infty} B(k)\sin(ku)\, k\, dk. \tag{9}$$

It is obvious that the presence of $B(k)$ dose not have any effect on the form of the initial wave function but it is responsible for the slope of the wave function at $v = 0$, and vice versa for $A(k)$. Moreover, a complete description of the problem would include the specification of both of these quantities. On the other hand, since we are interested to construct wave packets with classical properties, we need to assume a specific relationship between these coefficients. The prescription is that these coefficients have the same functional form [6, 7] *i.e.*

$$A(k) = B(k), \tag{10}$$

which results in the following wave packet

$$\begin{aligned} \Psi(u,v) &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} A(k)[\cos(ku)\cos(kv) \\ &+ i\sin(ku)\sin(kv)]\, dk. \end{aligned} \tag{11}$$

To completely determine the wave packet, we should specify $A(k)$. We can find $A(k)$ by choosing an appropriate initial wave function such as two Gaussians at $u = \pm d$

$$\Psi(u,0) = e^{-\alpha(u-d)^2} + e^{-\alpha(u+d)^2}. \tag{12}$$

This choice of initial condition, using inverse fourier transform, is related to

$$A(k) = \sqrt{\frac{2}{\alpha}}\, e^{-\frac{k^2}{4\alpha}} \cos(kd), \tag{13}$$

which gives

$$\begin{aligned} \Psi(u,v) &= \frac{1-i}{2}\Big(e^{-\alpha(u+v+d)^2} + e^{-\alpha(u+v-d)^2} \\ &+ ie^{-\alpha(u-v+d)^2} + ie^{-\alpha(u-v-d)^2}\Big). \end{aligned} \tag{14}$$

Figure 1 shows the initial wave function and its initial slope for $d = 4$ and $\alpha = 1$. Since, from Bohmian interpretation of the quantum mechanics, the initial derivative of the imaginary part of the wave packet corresponds to the initial classical velocity, the presence of a nonzero and appropriate form of $B(k)$ can be justified. The plot of the initial slope of the wave packet contains a negative and a positive peaks which correspond to a incoming or outgoing particle, respectively. Figure 2 shows the resulting wave packet for $d = 2$ and $\alpha = 1$. As it can be seen from the figure, this wave packet never disperses and strongly peaks on the classical trajectory. Moreover, the height of the crest of the wave packet, which from WKB approximation corresponds to the inverse velocity of the particle, is constant along the classical path. This behavior is in complete agreement with the classical picture. However, the square of the wave packet increases at the intersection points of the trajectories which correctly corresponds to the probability of two possible particle's directions of motion. Note that our choice of the expansion coefficients (13) corresponds to a free particle with a positive or negative momentum which is located initially at $u = \pm d$.

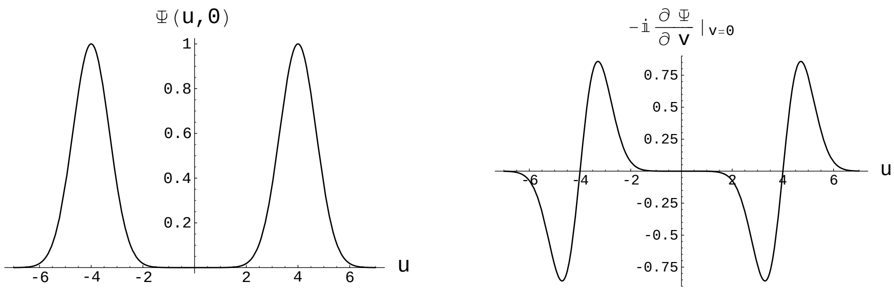

Figure 1: The initial wave function (left) and the initial derivative of the wave function (right) for $d = 4$ and $\alpha = 1$.

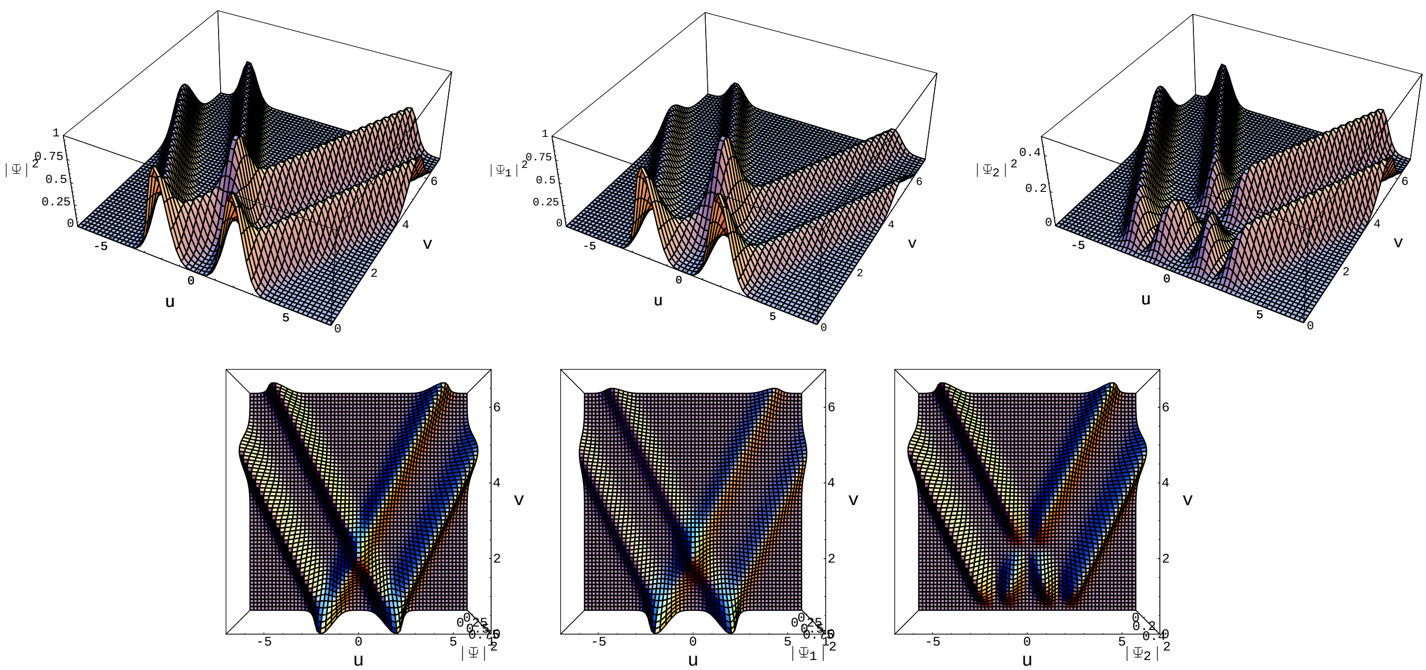

Figure 2: Up: the square of the wave packet $|\Psi(u,v)|^2$ (left), $[\mathrm{Re}[\Psi(u,v)]]^2$ (middle), and $[\mathrm{Im}[\Psi(u,v)]]^2$ (right) for $d = 2$ and $\alpha = 1$, Down: the respective upper view.

4 Particle in a box

For a particle in a box, we have

$$V(q) = \begin{cases} 0 & -\frac{L}{2} < q < \frac{L}{2}, \\ \infty & \text{otherwise}, \end{cases} \tag{15}$$

where q stands for u or v. For this case, the trajectories also are straight lines with unit absolute slope. Moreover, this model has well-known orthonormal even and odd eigenfunctions

$$\psi_n(q) = \begin{cases} \sqrt{\frac{2}{L}} \cos(\frac{n\pi q}{L}), & n = 1, 3, 5, ..., \\ \sqrt{\frac{2}{L}} \sin(\frac{n\pi q}{L}), & n = 2, 4, 6, ... \end{cases} \tag{16}$$

Now, using the exact form of the eigenstates, we find the following wave packet

$$\begin{aligned} \Psi(u, v) &= \sum_{n=1,3,5,...} A(n) \cos(\frac{n\pi u}{L}) \cos(\frac{n\pi v}{L}) \\ &+ i \sum_{n=2,4,6,...} A(n) \sin(\frac{n\pi u}{L}) \sin(\frac{n\pi v}{L}). \end{aligned} \tag{17}$$

If we demand that this solution satisfies the initial condition of Eq. (12), we obtain the following form of the expansion coefficients

$$\begin{aligned} A(n) &= \frac{-ie^{\frac{n\pi(n\pi+4i\alpha dL)}{4\alpha L^2}}}{L\sqrt{\alpha/\pi}} \left[-\text{Erfi}(\frac{n\pi + 2i\alpha L\,(d-L)}{2\sqrt{\alpha}L}) \right. \\ &+ e^{\frac{2idn\pi}{L}} \left(\text{Erfi}(\frac{n\pi - 2i\alpha L\,(d-L)}{2\sqrt{\alpha}L}) \right. \\ &- \left. \text{Erfi}(\frac{n\pi - 2i\alpha L\,(d+L)}{2\sqrt{\alpha}L}) \right) \\ &+ \left. \text{Erfi}(\frac{n\pi + 2i\alpha L\,(d+L)}{2\sqrt{\alpha}L}) \right], \end{aligned} \tag{18}$$

where $\text{Erfi}(x)$ is the imaginary error function $\text{Erfi}(x) \equiv -i\,\text{Erf}(ix)$. Figure 3 shows the wave packet for $d = 1.5$ and $\alpha = 5$. Classically, the particle is free inside the well and moves with positive or negative initial velocity from any arbitrary position in the range $-L/2 < u, v < L/2$. As it can seen from the figure, the wave packet follows the classical path and strongly peaks on it which is in complete agreement with the classical scenario. In fact, the value of d determines the initial classical position and the presence of two rectangles with opposite directions indicates the two possible directions of motion.

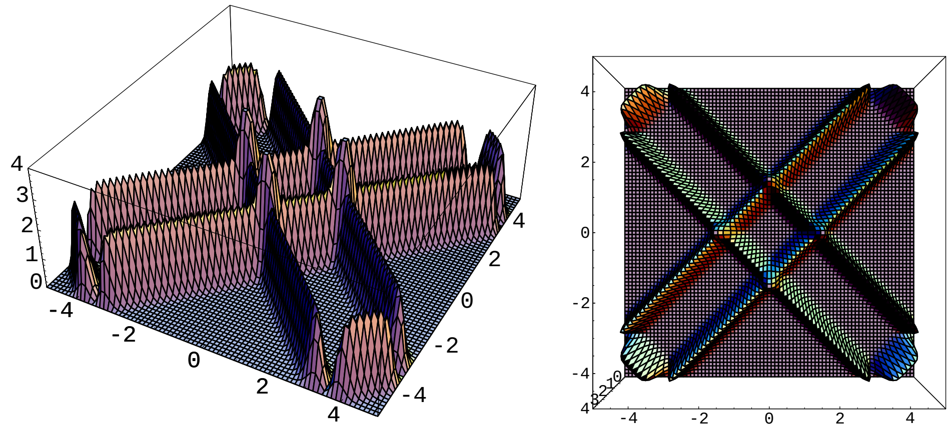

Figure 3: The square of the wave packet $|\Psi(u,v)|^2$ (left), and the respective upper view (right) for $d = 1.5$ and $\alpha = 5$.

Since the height of the crest of the wave packet is constant along the classical trajectory, the probability of finding the particle is constant along the classical path. On the other hand, since the classical velocity of the particle for this case is a constant of motion, the classical probability of finding the particle is also constant along its trajectory. So, the classical probability completely coincides with the quantum mechanical probability.

5 Classical limit, notion of time, uncertainty principle, and the conservation law

Now, we can define the classical wave packet which is nearly zero beyond the classical path as follows:

$$\Psi_{cl}(u,v) \equiv \lim_{\alpha\to\infty} \Psi(u,v). \tag{19}$$

This wave packet has the desired property $\Psi_{cl}(u,v) \neq 0$ at $\{u = u_{cl}, v = v_{cl}\}$ and $\Psi_{cl}(u,v) \simeq 0$ elsewhere. In fact, the wave packet does not disperse even for large values of α. This is in contrast with the solutions of the Schrödinger equation which usually disperses quickly as the particle moves.

The notion of time does not appear explicitly in our main equation (5). However, as we have shown, the results depend on time in an implicit manner. We also encounter this phenomenon in the context of quantum cosmology where its main equation, which is the Wheeler-DeWitt equation, does not contain time. Moreover, it is a hyperbolic differential equation and in particular conditions can be written in

the form of Eq. (5) [6]. Therefore, our approach can be considered as a bridge between relativistic and non–relativistic quantum mechanics. On the other hand, we can find the notion of time using the Bohmian interpretation of quantum mechanics, namely

$$p_\mu = \partial_\mu S, \tag{20}$$

where $\Psi = R\exp(iS)$. So, we can obtain the time evolution of each variable using this interpretation. Although this definition of time is not genuine, at the classical limit ($\alpha \to \infty$) it will coincide with the classical time as desired.

At this point, we encounter an important question: do these wave packets satisfy the Heisenberg uncertainty relation? For the case of a free particle, using the explicit form of the wave packet (14), we can check the uncertainty principle, for instance at $v = 0$. At this point, the uncertainties in u and p_u take the following form

$$\begin{aligned}(\Delta u)^2 &= \frac{1}{4\alpha} + \frac{d^2}{2}\left(1 + \tanh(d^2\alpha)\right) \\ &- \left(\frac{\sqrt{\frac{2}{\pi\alpha}} + d^2 e^{2d^2\alpha}\mathrm{Erf}(\sqrt{2\alpha}d^2)}{1 + e^{2d^2\alpha}}\right)^2, \end{aligned}\tag{21}$$

$$(\Delta p_u)^2 = \alpha\hbar^2\left[1 - \frac{4\alpha}{1 + e^{2d^2\alpha}}\left(d^2\alpha - \frac{2/\pi}{1 + e^{2d^2\alpha}}\right)\right], \tag{22}$$

where the integration is over $\{0, \infty\}$. Since the initial wave function contains two well-separated Gaussians located at $\pm d$ ($\alpha d^2 > 1$), we have $(\Delta u)^2 \simeq \frac{1}{4\alpha}$ and $(\Delta p_u)^2 \simeq \alpha\hbar^2$ which results in $(\Delta u)^2(\Delta p_u)^2 \simeq \hbar^2/4$. So, similar to the coherent states, the initial form of the wave packet satisfies the minimized uncertainty relation for all values of d and α subjected to $\alpha d^2 > 1$. Since the wave packet preserves its shape during the motion, we expect that this result also holds for other values of v.

Note that, in this formulation, the total probability at fixed u or v is not a conserved quantity. In fact, the wave packets which are solutions of the Eq. (5) satisfy the following conservation law

$$\partial_\mu J_\mu = 0, \tag{23}$$

where the probability current is defined as

$$J_\mu = \frac{\hbar^2}{2m}(\Psi^* \partial_\mu \Psi - \Psi \partial_\mu \Psi^*). \tag{24}$$

Therefore, the probability interpretation of Eq. (5) is similar to the Klein–Gordon equation.

6 Conclusions

In this paper, we have presented an alternative quantization procedure which results in a hyperbolic differential equation. We showed that, for the case of a free particle and a particle in a box, the structure of the underlying quantum mechanical equation and appropriate initial conditions led to complete classical–quantum correspondence. The wave packets never dispersed and followed the classical trajectories in the whole configuration space and strongly peaked on them.

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